A Semantic Technology for Materials Design and Development

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Description:
OBJECTIVE: Develop and demonstrate the foundational elements required to create a semantic technology for materials design and development. DESCRIPTION: Several foundational elements required to achieve Sir Tim Berners-Lee"s vision for a semantic web are in place and available to the materials community. The semantic web, sometimes referred to as the web-of-data, focuses on ontologies as well as the linking data for machine-to-machine data interchange (implemented via RDF and OWL). Linkage between multiple datasets, files and their respective metadata can be established in an ad hoc fashion without having to adhere to specific database table structures. Linked data without context is of limited value. A semantic web for materials requires common vocabularies. An example of a common vocabulary is the Dublin Core (DC) ontology, a set of universally accepted metadata used to describe a resource (e.g. document). The development and publishing of vocabulary using RDFS/OWL is one of the initial steps required to link relevant materials information across disparate (federated) sources. The development of common vocabularies could be jump-started by businesses via crowd sourcing and curated by materials subject matter experts (SME). Additionally, collaborative efforts with professional societies and other organizations (e.g. ASTM terminology standards, CEN, ASM, TMS, etc.) could be used to accelerate vocabulary/ontology development. Over time, multiple vocabularies would likely winnow down to key sets of generally accepted terms and mappings between terms having the same meaning. Taxonomies, a form of ontology, can express simple relationships in the materials domain. More sophisticated relationships between materials processing, structure and properties can be expressed using complex ontologies. These ontologies need to be developed and implemented using World Wide Web Consortium (W3C) recommendations like RDF/OWL or widely accepted semantic

technology standards such as time.owl and DC. As the above elements are being established on a larger scale, various forms of materials informatics could be developed to greatly expand the materials data and design space for the materials scientists and engineers. Success requires innovative approaches during the development of agents to query linked materials data, applications to mash-up and integrate data, and reasoning/inferencing engines specifically tailored to the materials domain. Machine learning and other innovative"data hungry"approaches to extract knowledge could be developed and applied for materials design. PHASE I: Develop a proof-of-concept for semantically linked materials data and information to include vocabularies/ontologies. Use these technologies to demonstrate sophisticated semantic queries for materials data and information. Develop approaches for increasing ontology richness, capturing provenance and ensuring appropriate access to restricted linked materials data (e.g. export controlled or Intellectual Property). Consider how the system could expand to accommodate manufacturing and component design. PHASE II: Develop a robust midlevel materials ontology ready for crowd sourcing and initial experimental research use. Explore more sophisticated low level ontologies. Significantly expand the size of or integration across data stores. Propose and demonstrate computational approaches for establishing provenance and processing restricted linked materials data and information. Provide examples of integration with manufacturing or component design domains. PHASE III: Use the Phase II work to fully develop an operational crowd sourcing materials ontology, linked-data capability to support the open materials research and development community. Develop linkages to manufacturing and component design domain. PRIVATE SECTOR COMMERCIAL POTENTIAL/DUAL-USE APPLICATIONS: There is a growing realization that that vast amounts of historical and future materials development data is a valuable untapped resource for materials design. Those who support the development of a linked materials data concept and develop the tools to organize, relate, digest and synthesize the vast amount of materials data will likely find a welcome demand for their products from the community of materials designers, product designers and manufacturers in both the private and public sectors.